



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID : 3CU1  
Title : Crystal Structure of 2:2:2 FGFR2D2:FGF1:SOS complex  
Authors : Guo, F.; Dakshinamurthy, R.; Thallapuranam, S.K.K.; Sakon, J.  
Deposited on : 2008-04-15  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

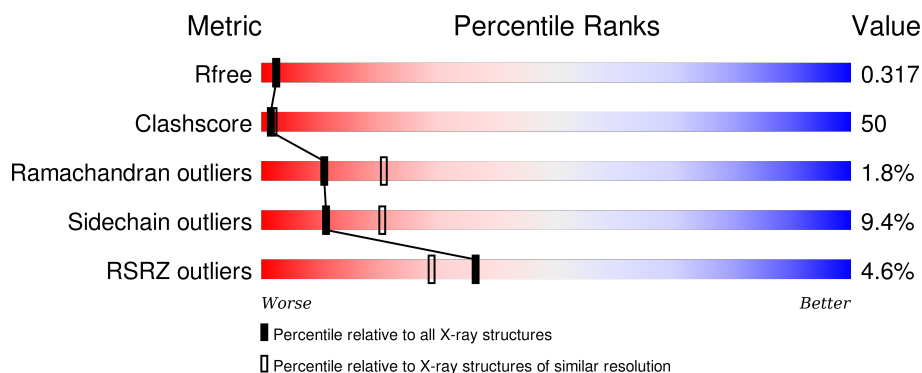
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	100	<div> <div>2%</div> <div>32% 44% 22%</div> </div>
1	C	100	<div> <div>2%</div> <div>33% 42% 23%</div> </div>
2	B	131	<div> <div>7%</div> <div>40% 31% 23%</div> </div>
2	D	131	<div> <div>6%</div> <div>30% 43% 20% 8%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4183 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

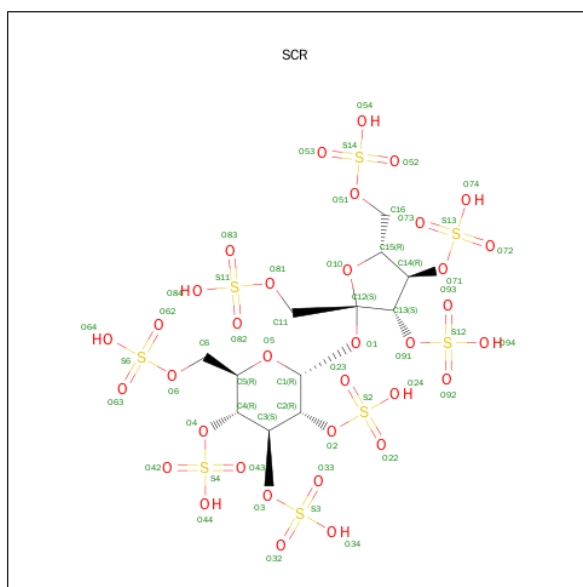
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	3	0
			832	524	157	145	6			
1	C	100	Total	C	N	O	S	0	2	0
			825	520	154	145	6			

- Molecule 2 is a protein called Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			1022	646	179	193	4			
2	D	131	Total	C	N	O	S	0	0	0
			1051	665	184	198	4			

- Molecule 3 is sucrose octasulfate (three-letter code: SCR) (formula:  $C_{12}H_{22}O_{35}S_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	O	S	0	0
			55	12	35	8		
3	B	1	Total	C	O	S	0	0
			55	12	35	8		

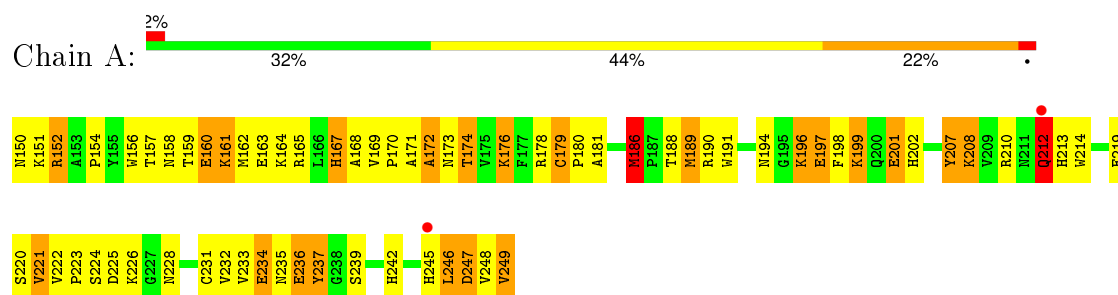
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	68	Total	O	0	0
			68	68		
4	C	98	Total	O	0	0
			98	98		
4	D	97	Total	O	0	0
			97	97		

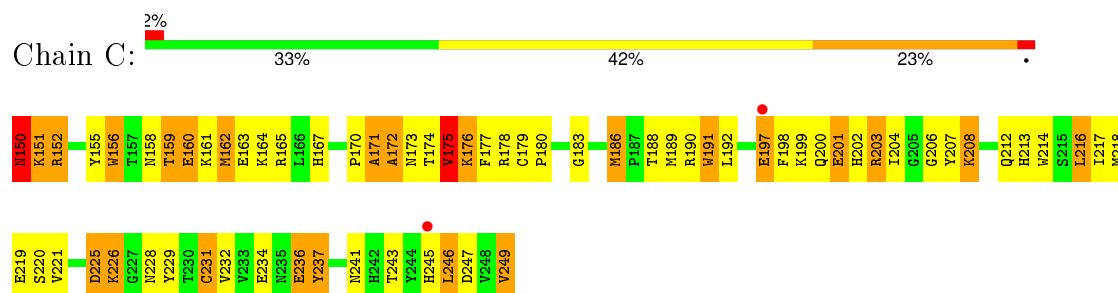
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

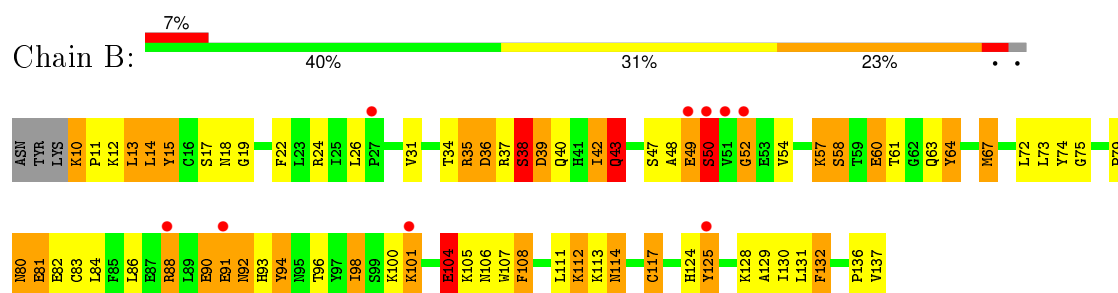
#### • Molecule 1: Fibroblast growth factor receptor 2



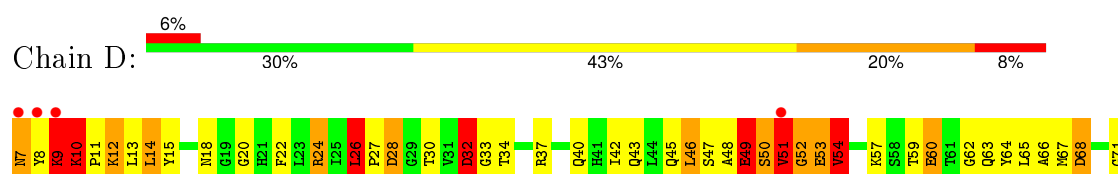
#### • Molecule 1: Fibroblast growth factor receptor 2

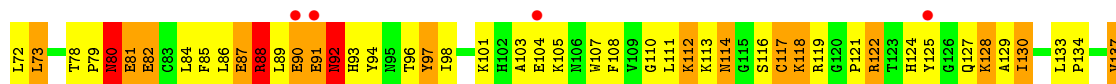


#### • Molecule 2: Heparin-binding growth factor 1



#### • Molecule 2: Heparin-binding growth factor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.93 Å 110.38 Å 74.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.95 – 2.60 35.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (42.95-2.60) 90.0 (35.38-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.24 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.277 0.261 , 0.317	Depositor DCC
$R_{free}$ test set	1044 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20263 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	2.74	63/868 (7.3%)	1.51	9/1173 (0.8%)
1	C	2.71	59/857 (6.9%)	1.52	11/1159 (0.9%)
2	B	2.23	40/1045 (3.8%)	1.41	15/1410 (1.1%)
2	D	2.46	45/1075 (4.2%)	1.56	21/1450 (1.4%)
All	All	2.52	207/3845 (5.4%)	1.50	56/5192 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	2	0

All (207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	117	CYS	CB-SG	-14.52	1.57	1.82
1	C	197	GLU	CG-CD	14.45	1.73	1.51
1	A	212[A]	GLN	CB-CG	12.71	1.86	1.52
1	A	212[B]	GLN	CB-CG	12.71	1.86	1.52
2	D	118	LYS	CE-NZ	12.13	1.79	1.49
1	C	197	GLU	CB-CG	11.88	1.74	1.52
2	D	81	GLU	CB-CG	-11.75	1.29	1.52
1	C	191	TRP	CE3-CZ3	11.49	1.57	1.38
1	C	175	VAL	CB-CG2	-11.38	1.28	1.52
2	D	104	GLU	CG-CD	11.02	1.68	1.51
2	B	125	TYR	CD1-CE1	10.62	1.55	1.39
2	D	87	GLU	CD-OE1	10.58	1.37	1.25
1	C	201	GLU	CB-CG	10.50	1.72	1.52
1	C	208	LYS	CB-CG	-10.50	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	128	LYS	CD-CE	10.47	1.77	1.51
1	A	160	GLU	CD-OE2	10.41	1.37	1.25
1	A	221	VAL	CB-CG2	-10.33	1.31	1.52
1	C	201	GLU	CG-CD	10.08	1.67	1.51
1	C	163	GLU	CD-OE1	9.98	1.36	1.25
1	A	219	GLU	CG-CD	9.77	1.66	1.51
1	A	196	LYS	CE-NZ	9.52	1.72	1.49
1	A	160	GLU	CG-CD	9.50	1.66	1.51
1	A	169	VAL	CB-CG1	-9.50	1.32	1.52
2	B	132	PHE	CE1-CZ	9.49	1.55	1.37
2	D	112	LYS	CD-CE	-9.30	1.28	1.51
1	C	171	ALA	CA-CB	-9.29	1.32	1.52
1	A	234	GLU	CD-OE1	9.16	1.35	1.25
1	C	236	GLU	CD-OE1	8.97	1.35	1.25
1	A	156	TRP	CZ3-CH2	-8.94	1.25	1.40
2	B	104	GLU	CD-OE1	8.85	1.35	1.25
1	A	237	TYR	CD1-CE1	-8.82	1.26	1.39
2	B	57	LYS	CE-NZ	8.75	1.71	1.49
2	D	87	GLU	CD-OE2	8.72	1.35	1.25
2	B	104	GLU	CG-CD	8.67	1.65	1.51
2	D	68	ASP	CB-CG	-8.48	1.33	1.51
1	A	219	GLU	CD-OE1	8.45	1.34	1.25
1	C	155	TYR	CD2-CE2	8.41	1.51	1.39
2	B	91	GLU	CG-CD	8.28	1.64	1.51
2	D	26	LEU	CG-CD2	8.19	1.82	1.51
2	B	94	TYR	CB-CG	-8.15	1.39	1.51
2	B	125	TYR	CE1-CZ	8.11	1.49	1.38
2	B	14	LEU	CG-CD1	-8.01	1.22	1.51
2	B	112	LYS	CE-NZ	7.97	1.69	1.49
1	C	218	MET	CB-CG	-7.94	1.25	1.51
1	A	197	GLU	CB-CG	-7.93	1.37	1.52
2	B	60	GLU	CB-CG	-7.88	1.37	1.52
1	A	207	TYR	CD2-CE2	-7.88	1.27	1.39
2	D	49	GLU	CB-CG	7.86	1.67	1.52
1	A	234	GLU	CG-CD	7.85	1.63	1.51
1	C	203	ARG	CG-CD	7.81	1.71	1.51
1	A	163	GLU	CD-OE2	7.79	1.34	1.25
1	A	197	GLU	CD-OE2	7.77	1.34	1.25
2	D	20	GLY	C-O	7.68	1.35	1.23
1	A	249	VAL	CB-CG1	-7.59	1.36	1.52
2	D	128	LYS	CE-NZ	7.58	1.68	1.49
1	C	160	GLU	CG-CD	7.51	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	ARG	CB-CG	-7.45	1.32	1.52
2	B	22	PHE	CB-CG	-7.39	1.38	1.51
1	C	176	LYS	CD-CE	7.34	1.69	1.51
1	A	190	ARG	CB-CG	-7.28	1.32	1.52
1	A	208	LYS	CD-CE	7.26	1.69	1.51
1	A	196	LYS	CD-CE	7.23	1.69	1.51
1	C	234	GLU	CG-CD	7.13	1.62	1.51
2	D	7	ASN	CB-CG	7.07	1.67	1.51
1	C	150	ASN	CB-CG	-7.06	1.34	1.51
1	C	191	TRP	CD2-CE2	7.06	1.49	1.41
1	A	234	GLU	CD-OE2	7.03	1.33	1.25
2	D	71	GLY	CA-C	-7.01	1.40	1.51
2	B	94	TYR	CE1-CZ	-7.00	1.29	1.38
2	D	88	ARG	CG-CD	6.98	1.69	1.51
1	C	172	ALA	CA-CB	-6.93	1.38	1.52
2	D	64	TYR	CB-CG	-6.91	1.41	1.51
2	D	87	GLU	CG-CD	6.88	1.62	1.51
1	A	248	VAL	CB-CG1	6.86	1.67	1.52
1	C	249	VAL	CB-CG2	6.85	1.67	1.52
2	D	137	VAL	CB-CG1	6.81	1.67	1.52
1	C	156	TRP	C-O	-6.81	1.10	1.23
2	B	91	GLU	C-O	-6.77	1.10	1.23
2	B	125	TYR	CG-CD2	6.75	1.48	1.39
1	C	203	ARG	CB-CG	-6.73	1.34	1.52
1	A	161	LYS	CD-CE	6.72	1.68	1.51
1	C	162	MET	N-CA	-6.71	1.32	1.46
2	B	10	LYS	CD-CE	6.71	1.68	1.51
1	A	161	LYS	CB-CG	6.70	1.70	1.52
2	D	49	GLU	CG-CD	6.70	1.62	1.51
1	A	163	GLU	CG-CD	6.70	1.61	1.51
1	C	191	TRP	CB-CG	-6.63	1.38	1.50
1	C	177	PHE	CD1-CE1	-6.60	1.26	1.39
1	A	207	TYR	CB-CG	-6.59	1.41	1.51
1	C	237	TYR	CD1-CE1	-6.54	1.29	1.39
1	A	201	GLU	CD-OE2	6.54	1.32	1.25
2	D	60	GLU	CD-OE1	6.52	1.32	1.25
1	A	236	GLU	CD-OE1	6.51	1.32	1.25
2	D	122	ARG	NE-CZ	6.45	1.41	1.33
1	A	150	ASN	CB-CG	-6.43	1.36	1.51
1	C	225	ASP	C-O	-6.42	1.11	1.23
1	C	163	GLU	CD-OE2	6.42	1.32	1.25
2	D	90	GLU	CB-CG	-6.42	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	49	GLU	CG-CD	6.39	1.61	1.51
1	A	237	TYR	CD2-CE2	-6.37	1.29	1.39
2	D	65	LEU	CA-CB	-6.36	1.39	1.53
2	B	64	TYR	CE1-CZ	6.36	1.46	1.38
1	C	170	PRO	CA-C	-6.36	1.40	1.52
1	A	232	VAL	CA-CB	-6.35	1.41	1.54
1	A	189	MET	CG-SD	6.33	1.97	1.81
2	D	82	GLU	C-O	6.32	1.35	1.23
2	D	73	LEU	C-O	6.29	1.35	1.23
1	A	161	LYS	CE-NZ	6.28	1.64	1.49
1	C	234	GLU	CD-OE1	6.28	1.32	1.25
1	C	231	CYS	CB-SG	-6.27	1.71	1.82
1	A	167	HIS	C-O	6.23	1.35	1.23
2	B	15	TYR	CD2-CE2	-6.23	1.30	1.39
2	D	128	LYS	CB-CG	6.19	1.69	1.52
2	D	117	CYS	CA-CB	-6.18	1.40	1.53
2	D	51	VAL	CA-CB	6.17	1.67	1.54
2	D	122	ARG	CD-NE	6.13	1.56	1.46
1	A	152	ARG	CG-CD	-6.12	1.36	1.51
1	C	243	THR	C-O	-6.12	1.11	1.23
2	D	15	TYR	CD2-CE2	-6.09	1.30	1.39
1	A	197	GLU	CG-CD	6.09	1.61	1.51
1	A	152	ARG	CZ-NH2	6.03	1.40	1.33
2	D	32	ASP	CB-CG	-6.03	1.39	1.51
1	C	246	LEU	CG-CD1	-6.01	1.29	1.51
1	C	198	PHE	CD2-CE2	5.99	1.51	1.39
1	A	224	SER	CA-CB	-5.98	1.44	1.52
2	B	49	GLU	CD-OE1	5.98	1.32	1.25
2	B	113	LYS	C-O	-5.98	1.11	1.23
2	B	24	ARG	CB-CG	-5.97	1.36	1.52
1	A	225	ASP	CG-OD1	5.97	1.39	1.25
1	C	172	ALA	N-CA	-5.94	1.34	1.46
1	A	181	ALA	CA-CB	-5.93	1.40	1.52
2	B	108	PHE	CE2-CZ	5.93	1.48	1.37
1	C	173	ASN	CG-OD1	-5.90	1.10	1.24
1	C	167	HIS	N-CA	-5.88	1.34	1.46
2	B	117	CYS	CB-SG	-5.88	1.72	1.81
1	A	160	GLU	CD-OE1	5.88	1.32	1.25
2	B	94	TYR	CZ-OH	-5.87	1.27	1.37
1	C	208	LYS	CD-CE	5.87	1.66	1.51
1	C	234	GLU	CB-CG	-5.86	1.41	1.52
1	C	207	TYR	CZ-OH	5.82	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	CD-OE2	5.78	1.32	1.25
1	A	198	PHE	CB-CG	-5.78	1.41	1.51
2	D	91	GLU	N-CA	-5.77	1.34	1.46
1	A	201	GLU	CD-OE1	5.77	1.31	1.25
2	B	64	TYR	C-O	5.76	1.34	1.23
1	C	186	MET	C-O	-5.73	1.12	1.23
1	A	247	ASP	CB-CG	-5.73	1.39	1.51
1	C	226	LYS	CD-CE	5.71	1.65	1.51
1	C	165	ARG	CZ-NH2	5.68	1.40	1.33
2	B	17	SER	CA-CB	-5.68	1.44	1.52
1	A	207	TYR	CD1-CE1	-5.68	1.30	1.39
1	A	172	ALA	N-CA	-5.67	1.35	1.46
2	B	38	SER	CB-OG	-5.66	1.34	1.42
2	B	90	GLU	CD-OE2	5.66	1.31	1.25
2	B	98	ILE	CA-CB	-5.65	1.41	1.54
1	C	165	ARG	CB-CG	-5.64	1.37	1.52
1	C	155	TYR	CE1-CZ	5.63	1.45	1.38
1	C	191	TRP	CD1-NE1	5.62	1.47	1.38
1	A	165	ARG	CG-CD	-5.62	1.38	1.51
1	C	201	GLU	CD-OE1	5.60	1.31	1.25
1	A	152	ARG	CA-CB	-5.59	1.41	1.53
2	D	90	GLU	CG-CD	5.57	1.60	1.51
1	A	201	GLU	CG-CD	5.51	1.60	1.51
1	C	152	ARG	CG-CD	5.51	1.65	1.51
1	A	247	ASP	CG-OD2	5.49	1.38	1.25
2	B	82	GLU	C-O	5.46	1.33	1.23
1	A	236	GLU	CD-OE2	5.45	1.31	1.25
1	C	175	VAL	CB-CG1	-5.44	1.41	1.52
2	B	35	ARG	CB-CG	-5.43	1.37	1.52
2	D	51	VAL	CB-CG2	5.43	1.64	1.52
1	C	151	LYS	CD-CE	5.41	1.64	1.51
1	C	229	TYR	CG-CD1	5.40	1.46	1.39
2	B	108	PHE	CD1-CE1	5.39	1.50	1.39
2	D	97	TYR	CG-CD2	5.38	1.46	1.39
1	C	176	LYS	CG-CD	5.37	1.70	1.52
2	D	81	GLU	CA-CB	-5.36	1.42	1.53
1	A	222	VAL	N-CA	5.35	1.57	1.46
1	C	190	ARG	CB-CG	-5.35	1.38	1.52
1	C	249	VAL	CB-CG1	-5.34	1.41	1.52
2	D	113	LYS	CB-CG	-5.34	1.38	1.52
1	A	235	ASN	CB-CG	-5.34	1.38	1.51
2	D	85	PHE	CE2-CZ	5.33	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	LYS	CD-CE	5.33	1.64	1.51
2	D	130	ILE	CA-CB	-5.31	1.42	1.54
1	A	176	LYS	CD-CE	5.30	1.64	1.51
2	B	74	TYR	CD2-CE2	5.27	1.47	1.39
1	C	249	VAL	N-CA	-5.27	1.35	1.46
2	B	91	GLU	CB-CG	5.27	1.62	1.52
1	A	162	MET	N-CA	-5.27	1.35	1.46
1	A	242	HIS	CA-C	-5.23	1.39	1.52
2	B	83	CYS	CB-SG	-5.23	1.73	1.81
1	C	165	ARG	CG-CD	-5.20	1.39	1.51
2	B	43	GLN	CA-CB	-5.20	1.42	1.53
1	C	183	GLY	CA-C	5.19	1.60	1.51
1	C	164	LYS	CE-NZ	5.18	1.62	1.49
2	B	88	ARG	CB-CG	-5.18	1.38	1.52
1	A	174	THR	CB-CG2	5.13	1.69	1.52
1	A	179	CYS	CA-CB	-5.12	1.42	1.53
2	D	14	LEU	C-O	5.11	1.33	1.23
1	A	247	ASP	CA-C	5.09	1.66	1.52
2	B	131	LEU	C-O	5.09	1.33	1.23
2	B	130	ILE	C-O	5.07	1.32	1.23
2	D	66	ALA	C-O	5.06	1.32	1.23
1	A	171	ALA	N-CA	5.05	1.56	1.46
2	D	88	ARG	NE-CZ	5.04	1.39	1.33
1	C	232	VAL	CA-CB	-5.04	1.44	1.54
2	D	52	GLY	N-CA	-5.03	1.38	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ASP	CB-CG-OD1	-10.22	109.10	118.30
2	D	68	ASP	CB-CA-C	-9.83	90.73	110.40
2	D	91	GLU	C-N-CA	8.80	143.71	121.70
2	D	51	VAL	N-CA-C	-8.67	87.59	111.00
2	D	32	ASP	N-CA-CB	-8.47	95.36	110.60
2	D	54	VAL	CB-CA-C	-7.92	96.36	111.40
2	D	117	CYS	CB-CA-C	-7.80	94.79	110.40
2	D	91	GLU	N-CA-C	7.74	131.90	111.00
2	D	91	GLU	CA-C-N	7.72	134.19	117.20
2	B	125	TYR	CA-CB-CG	7.65	127.94	113.40
1	C	165	ARG	NE-CZ-NH1	-7.65	116.48	120.30
1	A	190	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	C	151	LYS	N-CA-CB	-7.46	97.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	161	LYS	CD-CE-NZ	7.37	128.65	111.70
2	B	92	ASN	N-CA-C	7.35	130.84	111.00
2	D	26	LEU	CA-CB-CG	7.32	132.14	115.30
2	D	92	ASN	N-CA-CB	7.30	123.74	110.60
1	C	234	GLU	CB-CA-C	-7.29	95.81	110.40
2	B	36	ASP	CB-CG-OD1	7.13	124.71	118.30
2	B	117	CYS	CB-CA-C	-7.09	96.22	110.40
1	A	224	SER	CB-CA-C	-7.05	96.69	110.10
1	C	247	ASP	N-CA-CB	-6.80	98.36	110.60
1	A	210	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	B	125	TYR	CB-CA-C	6.35	123.10	110.40
1	A	247	ASP	CB-CG-OD2	6.25	123.92	118.30
1	C	190	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	204	ILE	CB-CA-C	6.24	124.08	111.60
2	B	13	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	C	203	ARG	CB-CA-C	-6.08	98.24	110.40
2	D	91	GLU	O-C-N	-6.05	113.03	122.70
2	B	111	LEU	CA-CB-CG	6.00	129.09	115.30
2	D	28	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	208	LYS	CB-CA-C	-5.90	98.61	110.40
2	B	88	ARG	N-CA-CB	-5.80	100.17	110.60
2	D	133	LEU	CB-CG-CD2	-5.76	101.20	111.00
2	D	84	LEU	CB-CG-CD1	-5.69	101.33	111.00
2	B	39	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	D	10	LYS	CB-CA-C	5.53	121.45	110.40
2	B	84	LEU	CB-CG-CD1	-5.48	101.68	111.00
2	D	53	GLU	N-CA-C	-5.47	96.23	111.00
2	D	32	ASP	CB-CG-OD1	-5.44	113.41	118.30
2	B	12	LYS	CB-CA-C	-5.39	99.61	110.40
2	B	38	SER	N-CA-CB	-5.39	102.41	110.50
2	D	24	ARG	CB-CG-CD	-5.37	97.65	111.60
2	B	125	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	D	92	ASN	CB-CA-C	5.20	120.81	110.40
2	D	46	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	234	GLU	CA-CB-CG	5.17	124.77	113.40
2	D	128	LYS	CD-CE-NZ	5.16	123.56	111.70
1	C	192	LEU	CB-CG-CD2	-5.11	102.32	111.00
2	B	39	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	186	MET	N-CA-CB	-5.08	101.45	110.60
1	C	162	MET	CB-CA-C	5.04	120.48	110.40
2	B	14	LEU	CB-CG-CD1	-5.02	102.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ARG	CB-CA-C	-5.01	100.37	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	91	GLU	CA
2	D	92	ASN	CA

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	832	0	810	58	0
1	C	825	0	801	86	0
2	B	1022	0	1007	90	0
2	D	1051	0	1035	137	0
3	B	55	0	21	6	0
3	D	55	0	20	18	0
4	A	80	0	0	26	0
4	B	68	0	0	32	0
4	C	98	0	0	32	0
4	D	97	0	0	48	0
All	All	4183	0	3694	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLU:CB	1:C:197:GLU:CG	1.74	1.63
2:D:128:LYS:NZ	2:D:128:LYS:CE	1.68	1.57
2:D:128:LYS:CE	2:D:128:LYS:CD	1.77	1.57
2:D:26:LEU:CD2	2:D:26:LEU:CG	1.82	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:LYS:CG	2:D:11:PRO:HD3	1.07	1.51
2:B:112:LYS:NZ	2:B:112:LYS:CE	1.69	1.51
2:B:57:LYS:CE	2:B:57:LYS:NZ	1.70	1.49
1:A:212[A]:GLN:CB	1:A:212[A]:GLN:CG	1.86	1.49
1:A:196:LYS:CE	1:A:196:LYS:NZ	1.72	1.48
2:D:10:LYS:HG2	2:D:11:PRO:CD	1.00	1.47
2:D:118:LYS:CE	2:D:118:LYS:NZ	1.79	1.45
1:A:186:MET:SD	1:A:186:MET:CE	2.05	1.45
1:C:200:GLN:HG2	4:C:375:HOH:O	1.40	1.22
2:D:51:VAL:HG12	4:D:210:HOH:O	1.38	1.19
1:A:179:CYS:HB2	4:A:323:HOH:O	1.44	1.18
1:C:174:THR:HB	4:C:361:HOH:O	1.02	1.17
2:B:47:SER:CB	4:B:210:HOH:O	1.93	1.17
1:C:216:LEU:HD23	1:C:217:ILE:N	1.59	1.16
2:D:101:LYS:HE2	4:D:222:HOH:O	1.46	1.15
2:B:48:ALA:HB1	2:B:50:SER:N	1.60	1.14
1:A:151:LYS:HD2	1:A:237:TYR:OH	1.46	1.14
1:C:220:SER:HB3	4:C:356:HOH:O	1.42	1.13
1:A:174:THR:HB	4:A:306:HOH:O	0.97	1.11
1:C:174:THR:HG22	4:C:358:HOH:O	1.49	1.11
2:D:87:GLU:HG3	2:D:97:TYR:CE2	1.84	1.11
2:B:81:GLU:HG3	2:B:101:LYS:HE2	1.32	1.11
2:D:137:VAL:O	4:D:211:HOH:O	1.68	1.09
1:C:171:ALA:HB3	4:C:372:HOH:O	0.92	1.08
2:B:124:HIS:HA	4:B:172:HOH:O	1.51	1.08
1:A:172:ALA:HB1	4:A:308:HOH:O	1.53	1.06
2:D:81:GLU:HA	4:D:269:HOH:O	1.56	1.06
2:B:47:SER:HB2	4:B:210:HOH:O	1.51	1.05
2:D:10:LYS:CD	2:D:11:PRO:HD2	1.86	1.05
2:D:118:LYS:NZ	3:D:1:SCR:O43	1.91	1.04
2:D:119:ARG:HD3	4:D:254:HOH:O	1.57	1.04
2:B:43:GLN:H	2:B:43:GLN:NE2	1.58	1.02
2:D:9:LYS:C	4:D:239:HOH:O	1.99	1.01
3:D:1:SCR:H162	4:D:258:HOH:O	1.58	1.01
2:D:86:LEU:HB3	2:D:88:ARG:HH22	1.23	1.00
2:B:48:ALA:HB1	2:B:50:SER:H	1.18	1.00
2:D:50:SER:HB3	2:D:51:VAL:HG22	1.00	0.99
2:B:43:GLN:HE21	2:B:43:GLN:N	1.60	0.98
2:D:50:SER:HB3	2:D:51:VAL:CG2	1.93	0.98
2:B:124:HIS:HB2	4:B:194:HOH:O	1.63	0.96
2:D:10:LYS:CG	2:D:11:PRO:CD	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:HE2	4:A:274:HOH:O	1.65	0.95
1:C:188:THR:HG23	4:C:289:HOH:O	1.65	0.95
1:C:216:LEU:C	1:C:216:LEU:CD2	2.34	0.94
2:D:125:TYR:CD2	4:D:206:HOH:O	2.18	0.94
2:D:10:LYS:CG	2:D:11:PRO:HD2	1.94	0.94
1:C:216:LEU:CD2	1:C:217:ILE:N	2.33	0.92
2:D:50:SER:CB	2:D:51:VAL:HG22	1.97	0.91
1:C:212[B]:GLN:OE1	4:C:381:HOH:O	1.87	0.91
1:C:216:LEU:C	1:C:216:LEU:HD23	1.88	0.89
2:D:10:LYS:CB	2:D:11:PRO:HD3	2.03	0.89
2:D:49:GLU:HA	2:D:50:SER:OG	1.73	0.89
1:C:150:ASN:N	4:C:380:HOH:O	2.04	0.89
1:C:174:THR:CB	4:C:361:HOH:O	1.76	0.88
2:D:9:LYS:HB2	4:D:240:HOH:O	1.72	0.87
1:C:151:LYS:HG2	1:C:237:TYR:CZ	2.08	0.87
2:D:90:GLU:HB3	2:D:92:ASN:HB2	1.56	0.87
2:D:86:LEU:HB3	2:D:88:ARG:NH2	1.87	0.87
2:D:10:LYS:CD	2:D:11:PRO:CD	2.47	0.87
1:A:197:GLU:HG2	4:A:272:HOH:O	1.74	0.86
2:D:60:GLU:HB2	4:D:185:HOH:O	1.76	0.86
2:D:134:PRO:HA	4:D:264:HOH:O	1.74	0.86
2:B:72:LEU:HD23	2:B:73:LEU:O	1.76	0.86
2:B:37:ARG:HD3	4:B:171:HOH:O	1.76	0.84
2:B:128:LYS:NZ	4:B:162:HOH:O	2.02	0.83
2:D:40:GLN:NE2	4:D:221:HOH:O	2.08	0.83
2:D:10:LYS:HG2	2:D:11:PRO:CG	2.05	0.82
2:D:10:LYS:N	4:D:239:HOH:O	2.12	0.81
2:B:47:SER:HB3	4:B:210:HOH:O	1.62	0.81
1:A:249:VAL:C	4:A:315:HOH:O	2.18	0.81
1:C:216:LEU:HD23	1:C:217:ILE:H	1.46	0.81
2:B:43:GLN:H	2:B:43:GLN:HE21	0.83	0.81
2:B:43:GLN:NE2	2:B:43:GLN:N	2.22	0.80
2:B:92:ASN:HB3	2:B:94:TYR:HD2	1.44	0.80
1:A:176:LYS:HE2	3:D:1:SCR:C11	2.12	0.79
2:B:49:GLU:HB3	4:B:197:HOH:O	1.81	0.79
2:D:11:PRO:O	2:D:137:VAL:HG23	1.83	0.79
1:C:150:ASN:HA	4:C:380:HOH:O	1.82	0.78
2:D:9:LYS:CA	4:D:239:HOH:O	2.29	0.77
1:C:172:ALA:HB1	4:C:376:HOH:O	1.83	0.77
2:D:37:ARG:NH2	4:D:215:HOH:O	2.07	0.77
2:D:14:LEU:HA	4:D:264:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:LEU:HD23	2:D:27:PRO:HD2	1.68	0.76
1:A:196:LYS:HB2	4:A:325:HOH:O	1.86	0.76
2:D:45:GLN:HG2	2:D:59:THR:HG22	1.66	0.76
1:C:179:CYS:HB2	4:C:309:HOH:O	1.86	0.76
2:D:10:LYS:HG2	2:D:11:PRO:HD2	1.47	0.75
3:D:1:SCR:O94	4:D:259:HOH:O	2.02	0.75
2:B:37:ARG:HG2	4:B:212:HOH:O	1.86	0.75
2:B:58:SER:OG	2:B:61:THR:HG22	1.86	0.75
1:C:151:LYS:HG2	1:C:237:TYR:CE2	2.21	0.74
3:D:1:SCR:H162	4:D:250:HOH:O	1.88	0.73
1:C:220:SER:CB	4:C:356:HOH:O	2.12	0.73
2:D:24:ARG:NH2	2:D:32:ASP:OD1	2.22	0.73
1:C:174:THR:CG2	4:C:358:HOH:O	2.20	0.73
2:D:10:LYS:HD3	2:D:11:PRO:HD2	1.69	0.72
2:B:93:HIS:HD2	4:B:152:HOH:O	1.70	0.72
1:A:199:LYS:HD3	1:A:202:HIS:CE1	2.24	0.72
1:A:207:TYR:CZ	4:A:298:HOH:O	2.43	0.72
2:D:122:ARG:HD3	3:D:1:SCR:O62	1.89	0.72
2:B:48:ALA:CB	2:B:50:SER:H	2.01	0.72
2:B:137:VAL:O	4:B:151:HOH:O	2.07	0.72
1:A:164:LYS:CE	4:A:274:HOH:O	2.30	0.71
2:B:37:ARG:CG	4:B:211:HOH:O	2.38	0.71
2:D:134:PRO:O	4:D:265:HOH:O	2.09	0.70
2:D:26:LEU:HG	2:D:26:LEU:CD2	2.16	0.70
2:B:19:GLY:O	2:B:35:ARG:NH2	2.23	0.70
2:D:9:LYS:HA	4:D:239:HOH:O	1.88	0.70
1:C:171:ALA:HB1	1:C:221:VAL:O	1.91	0.70
2:B:124:HIS:CD2	4:B:155:HOH:O	2.44	0.70
2:B:37:ARG:CD	4:B:211:HOH:O	2.40	0.70
2:D:118:LYS:NZ	3:D:1:SCR:S4	2.63	0.69
2:B:57:LYS:HD2	4:B:168:HOH:O	1.91	0.69
1:C:174:THR:O	1:C:174:THR:HG23	1.92	0.69
1:A:207:TYR:CE2	4:A:298:HOH:O	2.44	0.69
1:C:208:LYS:CE	4:C:297:HOH:O	2.40	0.69
2:D:114:ASN:ND2	2:D:116:SER:H	1.91	0.69
2:B:50:SER:OG	2:B:52:GLY:N	2.25	0.69
2:D:82:GLU:HG3	4:D:203:HOH:O	1.92	0.69
2:B:48:ALA:HB1	2:B:49:GLU:C	2.13	0.69
2:D:57:LYS:HE2	2:D:62:GLY:HA2	1.75	0.69
1:A:176:LYS:HE2	3:D:1:SCR:H112	1.74	0.68
1:C:150:ASN:N	1:C:150:ASN:OD1	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HD3	4:B:212:HOH:O	1.93	0.68
2:B:124:HIS:HD2	4:B:155:HOH:O	1.76	0.68
2:D:79:PRO:O	2:D:80:ASN:CB	2.41	0.68
2:D:89:LEU:HD21	4:D:193:HOH:O	1.94	0.68
2:D:118:LYS:NZ	3:D:1:SCR:H61	2.10	0.67
2:B:114:ASN:HD22	2:B:114:ASN:C	1.98	0.67
2:B:18:ASN:HB2	2:B:129:ALA:HA	1.76	0.67
1:C:208:LYS:HE2	4:C:297:HOH:O	1.96	0.66
2:B:125:TYR:HB3	4:B:154:HOH:O	1.95	0.66
1:C:199:LYS:HE3	4:C:327:HOH:O	1.95	0.66
2:D:87:GLU:HG3	2:D:97:TYR:HE2	1.57	0.66
1:C:156:TRP:CG	1:C:162:MET:HE2	2.31	0.66
2:D:114:ASN:C	2:D:114:ASN:HD22	1.99	0.66
1:C:175:VAL:CG2	1:C:221:VAL:HG21	2.25	0.66
2:D:18:ASN:HB2	2:D:129:ALA:HA	1.78	0.66
2:B:37:ARG:CD	4:B:212:HOH:O	2.43	0.65
2:D:88:ARG:HH21	2:D:88:ARG:HG2	1.62	0.65
2:D:8:TYR:O	2:D:12:LYS:HE2	1.97	0.65
2:D:90:GLU:HG3	2:D:91:GLU:H	1.62	0.65
2:D:45:GLN:HG2	2:D:59:THR:CG2	2.26	0.65
2:D:8:TYR:O	2:D:12:LYS:CE	2.45	0.64
2:D:125:TYR:HD2	4:D:206:HOH:O	1.66	0.64
1:C:216:LEU:C	1:C:216:LEU:HD22	2.14	0.64
2:B:72:LEU:CD2	2:B:73:LEU:O	2.44	0.64
2:B:104:GLU:OE2	2:B:105:LYS:HD3	1.98	0.64
1:A:213:HIS:HD2	4:D:249:HOH:O	1.79	0.64
1:C:150:ASN:CA	4:C:380:HOH:O	2.35	0.63
1:C:156:TRP:CZ3	1:C:179:CYS:HB3	2.32	0.63
2:D:48:ALA:HB1	2:D:49:GLU:HA	1.79	0.63
2:D:86:LEU:CB	2:D:88:ARG:HH22	2.06	0.63
2:B:37:ARG:HA	4:B:211:HOH:O	1.97	0.63
2:D:48:ALA:HB1	2:D:50:SER:HA	1.80	0.63
2:D:14:LEU:HD23	4:D:264:HOH:O	1.98	0.63
1:A:161:LYS:HE3	1:A:178[A]:ARG:HD2	1.80	0.62
2:D:43:GLN:HB3	4:D:246:HOH:O	1.99	0.62
2:B:48:ALA:HB1	2:B:49:GLU:CA	2.30	0.62
1:A:172:ALA:CB	4:A:308:HOH:O	2.24	0.62
2:B:37:ARG:CG	4:B:212:HOH:O	2.46	0.62
2:B:104:GLU:N	2:B:104:GLU:OE1	2.33	0.62
2:B:42:ILE:HD13	2:B:42:ILE:H	1.64	0.62
2:D:12:LYS:N	2:D:12:LYS:HD2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HD2	4:B:211:HOH:O	2.00	0.61
2:D:52:GLY:HA2	4:D:210:HOH:O	1.98	0.61
2:B:92:ASN:HB3	2:B:94:TYR:CD2	2.30	0.61
2:D:7:ASN:CG	2:D:8:TYR:H	2.04	0.61
2:D:114:ASN:HD22	2:D:116:SER:H	1.48	0.61
1:C:220:SER:CA	4:C:356:HOH:O	2.44	0.61
1:C:156:TRP:CD2	1:C:162:MET:HE2	2.36	0.61
2:D:122:ARG:HD2	4:D:262:HOH:O	2.00	0.60
1:C:152:ARG:HG2	4:C:371:HOH:O	2.01	0.60
2:D:18:ASN:ND2	2:D:129:ALA:HB2	2.16	0.60
2:B:61:THR:HG23	2:B:63:GLN:HG3	1.83	0.60
2:D:43:GLN:CB	4:D:246:HOH:O	2.50	0.59
1:C:201:GLU:HA	4:C:323:HOH:O	2.01	0.59
3:B:1:SCR:O92	1:C:161:LYS:NZ	2.35	0.59
2:B:43:GLN:HG2	4:B:209:HOH:O	2.02	0.58
2:B:37:ARG:HG3	4:B:211:HOH:O	2.00	0.58
1:C:197:GLU:O	1:C:202:HIS:HE1	1.87	0.58
1:A:197:GLU:HA	4:A:272:HOH:O	2.02	0.58
1:C:191:TRP:CE2	1:C:216:LEU:HB2	2.38	0.58
2:D:101:LYS:HD3	4:D:270:HOH:O	2.04	0.58
2:D:101:LYS:HG3	4:D:217:HOH:O	2.03	0.58
2:D:124:HIS:CE1	2:D:127:GLN:NE2	2.72	0.58
2:D:78:THR:HG23	4:D:220:HOH:O	2.02	0.57
1:C:156:TRP:CD2	1:C:162:MET:CE	2.87	0.57
3:B:1:SCR:O53	3:B:1:SCR:H15	2.02	0.57
1:A:228:ASN:CB	4:A:316:HOH:O	2.53	0.57
2:D:98:ILE:HD11	2:D:108:PHE:CE2	2.40	0.57
2:B:105:LYS:HE3	2:B:107:TRP:CZ2	2.40	0.57
1:A:168:ALA:HB3	2:B:15:TYR:CE2	2.40	0.57
2:B:81:GLU:HB2	2:B:101:LYS:HD3	1.86	0.57
2:D:107:TRP:CZ2	2:D:121:PRO:HG3	2.40	0.56
2:D:88:ARG:NH2	2:D:88:ARG:HG2	2.19	0.56
2:D:57:LYS:CE	2:D:62:GLY:HA2	2.36	0.56
2:D:122:ARG:NH1	4:D:207:HOH:O	2.30	0.56
1:A:207:TYR:CD2	1:A:207:TYR:C	2.79	0.56
2:D:49:GLU:HA	2:D:50:SER:CB	2.34	0.56
2:D:111:LEU:HD23	2:D:117:CYS:HA	1.87	0.56
1:A:154:PRO:O	4:A:250:HOH:O	2.18	0.56
2:B:14:LEU:N	2:B:14:LEU:HD12	2.21	0.55
2:D:47:SER:O	2:D:54:VAL:HA	2.06	0.55
2:D:90:GLU:HG3	2:D:91:GLU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:THR:CG2	4:C:355:HOH:O	2.54	0.55
1:C:151:LYS:HE3	1:C:237:TYR:OH	2.06	0.55
2:D:46:LEU:HB3	2:D:54:VAL:HG11	1.88	0.55
2:D:87:GLU:CG	2:D:97:TYR:CE2	2.76	0.55
1:C:171:ALA:CB	4:C:372:HOH:O	1.80	0.55
3:B:1:SCR:H61	3:B:1:SCR:S4	2.47	0.55
1:A:188:THR:HG22	1:A:189:MET:N	2.21	0.55
1:A:233:VAL:O	1:A:239:SER:HA	2.07	0.54
1:C:171:ALA:CB	1:C:221:VAL:O	2.55	0.54
1:C:228:ASN:OD1	1:C:245[B]:HIS:HD2	1.90	0.54
1:C:156:TRP:HZ3	1:C:179:CYS:HB3	1.73	0.54
1:A:228:ASN:HB3	4:A:316:HOH:O	2.08	0.54
2:B:36:ASP:OD1	2:B:38:SER:HB3	2.07	0.54
2:D:81:GLU:HB3	4:D:203:HOH:O	2.06	0.54
3:B:1:SCR:H5	3:B:1:SCR:O10	2.08	0.53
1:A:176:LYS:HD3	1:A:178[A]:ARG:HH21	1.73	0.53
2:D:134:PRO:HD2	4:D:265:HOH:O	2.08	0.53
2:B:137:VAL:O	2:B:137:VAL:HG12	2.09	0.53
2:D:79:PRO:O	2:D:80:ASN:HB2	2.08	0.53
1:C:175:VAL:HG23	1:C:221:VAL:HG21	1.91	0.53
1:C:151:LYS:CE	1:C:237:TYR:OH	2.57	0.52
1:A:161:LYS:HE3	1:A:178[B]:ARG:HD3	1.90	0.52
1:C:189:MET:CE	1:C:191:TRP:HE1	2.22	0.52
1:A:178[B]:ARG:NH1	1:A:180:PRO:HG3	2.24	0.52
1:C:174:THR:OG1	4:C:361:HOH:O	2.05	0.52
1:A:236:GLU:OE1	1:A:236:GLU:N	2.39	0.52
2:B:88:ARG:HH21	2:B:88:ARG:HG3	1.75	0.52
1:A:208:LYS:HG3	4:A:307:HOH:O	2.09	0.52
2:D:128:LYS:CE	2:D:128:LYS:CG	2.81	0.51
2:D:78:THR:CG2	4:D:220:HOH:O	2.57	0.51
1:C:159:THR:HG22	4:C:355:HOH:O	2.10	0.51
1:C:151:LYS:CG	1:C:237:TYR:OH	2.58	0.51
1:C:158:ASN:C	1:C:158:ASN:OD1	2.46	0.51
2:D:92:ASN:HB3	2:D:94:TYR:H	1.75	0.51
2:D:89:LEU:HD11	2:D:93:HIS:HB3	1.92	0.51
1:A:180:PRO:HB3	1:C:160:GLU:OE2	2.10	0.51
2:B:49:GLU:HG2	2:B:50:SER:O	2.10	0.51
2:D:13:LEU:HD22	2:D:42:ILE:HG13	1.92	0.51
2:B:112:LYS:CD	2:B:112:LYS:NZ	2.61	0.51
2:B:67:MET:HG3	2:B:73:LEU:HD23	1.93	0.51
2:D:28:ASP:OD1	2:D:30:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:VAL:O	2:D:137:VAL:HG12	2.11	0.51
2:D:90:GLU:HB3	2:D:92:ASN:CB	2.37	0.51
2:D:137:VAL:C	4:D:209:HOH:O	2.50	0.50
1:C:191:TRP:CZ3	1:C:231:CYS:HB3	2.46	0.50
1:C:197:GLU:O	1:C:202:HIS:CE1	2.65	0.50
2:D:51:VAL:CG1	4:D:210:HOH:O	2.20	0.50
1:A:246:LEU:HD22	1:A:247:ASP:N	2.27	0.50
1:A:158:ASN:N	4:A:309:HOH:O	2.31	0.50
2:D:137:VAL:O	4:D:209:HOH:O	2.20	0.50
3:D:1:SCR:O34	3:D:1:SCR:S4	2.69	0.50
2:B:37:ARG:CD	4:B:171:HOH:O	2.48	0.50
1:C:180:PRO:HA	1:C:214:TRP:CD1	2.48	0.49
1:A:176:LYS:HD3	3:D:1:SCR:O24	2.13	0.49
2:D:48:ALA:CB	2:D:49:GLU:HA	2.42	0.49
2:D:88:ARG:HH21	2:D:88:ARG:CG	2.24	0.49
2:B:114:ASN:C	2:B:114:ASN:ND2	2.64	0.49
3:B:1:SCR:O83	3:B:1:SCR:H62	2.13	0.49
1:C:176:LYS:NZ	4:C:365:HOH:O	2.44	0.49
1:A:151:LYS:HB3	1:A:237:TYR:CE2	2.47	0.49
2:D:11:PRO:O	2:D:137:VAL:CG2	2.57	0.49
2:D:49:GLU:CA	2:D:50:SER:OG	2.55	0.49
2:D:98:ILE:HG12	2:D:108:PHE:CD2	2.48	0.49
2:D:122:ARG:HD3	3:D:1:SCR:S6	2.53	0.48
2:D:49:GLU:OE2	2:D:49:GLU:O	2.31	0.48
2:B:136:PRO:HD2	4:B:142:HOH:O	2.13	0.48
1:C:151:LYS:CG	1:C:237:TYR:CZ	2.91	0.48
2:B:92:ASN:HB2	2:B:94:TYR:H	1.78	0.48
2:B:13:LEU:HD22	2:B:42:ILE:HG12	1.95	0.48
2:D:117:CYS:CB	4:D:257:HOH:O	2.61	0.48
2:D:47:SER:H	2:D:54:VAL:HG12	1.78	0.48
1:C:226:LYS:HG2	4:C:344:HOH:O	2.13	0.48
2:D:118:LYS:HZ2	3:D:1:SCR:H61	1.78	0.48
2:B:47:SER:O	2:B:54:VAL:HA	2.13	0.48
2:D:101:LYS:HB2	4:D:251:HOH:O	2.13	0.48
1:C:203:ARG:NH1	1:C:206:GLY:O	2.43	0.48
2:D:124:HIS:NE2	2:D:127:GLN:NE2	2.60	0.48
2:D:49:GLU:HG2	2:D:50:SER:HB2	1.95	0.47
2:D:40:GLN:O	2:D:60:GLU:HG3	2.13	0.47
2:D:114:ASN:ND2	2:D:116:SER:OG	2.41	0.47
2:B:90:GLU:C	2:B:92:ASN:H	2.17	0.47
2:D:112:LYS:HG2	3:D:1:SCR:O44	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:THR:O	1:C:174:THR:CG2	2.59	0.47
1:C:188:THR:HB	4:C:373:HOH:O	2.14	0.47
2:D:114:ASN:ND2	2:D:114:ASN:C	2.68	0.47
1:C:158:ASN:OD1	1:C:158:ASN:O	2.32	0.47
2:D:67:MET:HB3	4:D:224:HOH:O	2.13	0.47
1:C:236:GLU:HG2	4:C:300:HOH:O	2.15	0.47
2:B:79:PRO:O	2:B:80:ASN:CB	2.61	0.47
2:B:93:HIS:CD2	4:B:152:HOH:O	2.56	0.46
1:A:188:THR:CG2	1:A:189:MET:N	2.78	0.46
1:A:191:TRP:CH2	1:A:231:CYS:HB3	2.50	0.46
1:C:152:ARG:CG	4:C:371:HOH:O	2.59	0.46
2:D:32:ASP:OD2	2:D:33:GLY:N	2.48	0.46
2:B:48:ALA:HB1	2:B:49:GLU:HA	1.97	0.46
2:B:11:PRO:O	2:B:137:VAL:HG23	2.16	0.46
1:C:151:LYS:HG2	1:C:237:TYR:OH	2.16	0.46
2:D:8:TYR:O	2:D:12:LYS:HE3	2.16	0.46
2:B:64:TYR:O	2:B:75:GLY:HA2	2.15	0.46
1:A:170:PRO:HD2	1:A:173:ASN:HD22	1.80	0.46
1:C:203:ARG:NH2	1:C:219:GLU:O	2.44	0.46
2:B:91:GLU:CG	4:B:193:HOH:O	2.64	0.45
3:D:1:SCR:C16	4:D:258:HOH:O	2.36	0.45
2:B:48:ALA:CB	2:B:50:SER:N	2.54	0.45
2:B:15:TYR:O	2:B:132:PHE:HA	2.17	0.45
2:B:91:GLU:HG3	4:B:193:HOH:O	2.16	0.45
1:C:172:ALA:HA	4:C:351:HOH:O	2.15	0.45
2:D:117:CYS:HB2	4:D:257:HOH:O	2.16	0.45
2:B:88:ARG:HB3	2:B:96:THR:OG1	2.16	0.45
1:C:246:LEU:HD12	1:C:246:LEU:HA	1.64	0.45
1:A:157:THR:HB	1:C:159:THR:HG22	1.99	0.45
1:C:213:HIS:O	1:C:214:TRP:HB2	2.17	0.45
2:B:90:GLU:O	2:B:92:ASN:N	2.44	0.45
2:D:12:LYS:N	2:D:12:LYS:CD	2.80	0.45
1:A:245[B]:HIS:CD2	4:A:265:HOH:O	2.69	0.45
1:C:191:TRP:CH2	1:C:231:CYS:HB3	2.52	0.45
1:C:156:TRP:CE2	1:C:162:MET:HE1	2.52	0.45
1:C:249:VAL:C	4:C:357:HOH:O	2.54	0.45
1:C:175:VAL:HG23	1:C:221:VAL:CG2	2.47	0.44
2:D:45:GLN:CG	2:D:59:THR:HG22	2.43	0.44
1:A:158:ASN:C	4:A:309:HOH:O	2.56	0.44
2:B:40:GLN:HG3	4:B:182:HOH:O	2.17	0.44
1:A:234:GLU:HB3	1:A:239:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ALA:HA	2:D:53:GLU:O	2.17	0.44
1:C:178:ARG:NH2	1:C:180:PRO:HG3	2.31	0.44
2:D:118:LYS:CE	3:D:1:SCR:H61	2.48	0.44
2:B:105:LYS:HE2	2:B:105:LYS:HB2	1.57	0.44
3:B:1:SCR:H112	3:B:1:SCR:H1	1.72	0.43
1:C:225:ASP:O	1:C:226:LYS:C	2.56	0.43
1:A:199:LYS:HB3	4:A:318:HOH:O	2.17	0.43
2:D:43:GLN:N	2:D:43:GLN:OE1	2.45	0.43
1:A:159:THR:O	1:A:160:GLU:C	2.57	0.43
2:D:110:GLY:N	4:D:190:HOH:O	2.45	0.43
3:D:1:SCR:O34	3:D:1:SCR:O42	2.36	0.43
1:A:164:LYS:HD3	1:A:167:HIS:NE2	2.34	0.42
3:D:1:SCR:O71	4:D:247:HOH:O	2.21	0.42
2:B:48:ALA:CB	2:B:49:GLU:CA	2.96	0.42
2:B:26:LEU:HG	4:B:207:HOH:O	2.19	0.42
2:D:68:ASP:OD1	2:D:72:LEU:HB3	2.19	0.42
2:B:92:ASN:CB	2:B:94:TYR:HD2	2.23	0.42
1:A:223:PRO:HD2	4:A:313:HOH:O	2.20	0.42
1:A:172:ALA:O	1:A:220:SER:HA	2.19	0.42
1:C:156:TRP:CD2	1:C:162:MET:HE1	2.53	0.42
1:A:208:LYS:CE	4:A:307:HOH:O	2.67	0.42
1:A:194:ASN:HA	4:A:275:HOH:O	2.19	0.42
2:B:98:ILE:HD11	2:B:108:PHE:CE2	2.55	0.41
2:B:106:ASN:HD22	2:B:106:ASN:HA	1.69	0.41
2:D:103:ALA:C	2:D:105:LYS:H	2.24	0.41
2:B:34:THR:HA	4:B:195:HOH:O	2.20	0.41
1:A:152:ARG:HG3	4:A:260:HOH:O	2.19	0.41
2:D:48:ALA:C	4:D:241:HOH:O	2.58	0.41
2:D:14:LEU:CD2	4:D:264:HOH:O	2.62	0.41
1:A:189:MET:CE	1:A:214:TRP:C	2.88	0.41
2:B:92:ASN:CB	2:B:94:TYR:H	2.33	0.41
1:C:226:LYS:HB2	1:C:226:LYS:HE2	1.53	0.41
2:D:72:LEU:HD12	2:D:73:LEU:N	2.35	0.41
2:B:31:VAL:O	2:B:117:CYS:SG	2.79	0.41
2:D:96:THR:HG22	2:D:130:ILE:O	2.21	0.41
1:A:208:LYS:CD	4:A:307:HOH:O	2.68	0.41
2:D:14:LEU:O	2:D:22:PHE:HA	2.20	0.41
1:A:208:LYS:HE3	4:A:307:HOH:O	2.21	0.41
2:B:86:LEU:HD21	2:B:100:LYS:HD3	2.02	0.41
2:B:10:LYS:HB3	2:B:10:LYS:HE3	1.78	0.40
2:B:128:LYS:HD2	2:B:128:LYS:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LYS:HB3	1:C:199:LYS:HE2	1.86	0.40
1:C:180:PRO:HA	1:C:214:TRP:CG	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/100 (101%)	98 (97%)	3 (3%)	0	100	100
1	C	100/100 (100%)	93 (93%)	7 (7%)	0	100	100
2	B	126/131 (96%)	113 (90%)	11 (9%)	2 (2%)	12	24
2	D	129/131 (98%)	114 (88%)	9 (7%)	6 (5%)	3	3
All	All	456/462 (99%)	418 (92%)	30 (7%)	8 (2%)	11	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	10	LYS
2	D	92	ASN
2	B	52	GLY
2	D	50	SER
2	D	80	ASN
2	D	9	LYS
2	B	50	SER
2	D	12	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/88 (103%)	83 (91%)	8 (9%)	12	24
1	C	90/88 (102%)	84 (93%)	6 (7%)	20	40
2	B	112/115 (97%)	99 (88%)	13 (12%)	7	12
2	D	115/115 (100%)	103 (90%)	12 (10%)	9	16
All	All	408/406 (100%)	369 (90%)	39 (10%)	11	20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	MET
1	A	199	LYS
1	A	201	GLU
1	A	212[A]	GLN
1	A	212[B]	GLN
1	A	221	VAL
1	A	226	LYS
1	A	246	LEU
2	B	38	SER
2	B	39	ASP
2	B	42	ILE
2	B	43	GLN
2	B	50	SER
2	B	58	SER
2	B	60	GLU
2	B	67	MET
2	B	80	ASN
2	B	81	GLU
2	B	101	LYS
2	B	104	GLU
2	B	114	ASN
1	C	150	ASN
1	C	159	THR
1	C	175	VAL
1	C	186	MET
1	C	216	LEU
1	C	241	ASN
2	D	9	LYS

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Mol	Chain	Res	Type
2	D	10	LYS
2	D	26	LEU
2	D	32	ASP
2	D	34	THR
2	D	49	GLU
2	D	51	VAL
2	D	54	VAL
2	D	63	GLN
2	D	80	ASN
2	D	88	ARG
2	D	114	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	43	GLN
2	B	102	HIS
2	B	106	ASN
2	B	114	ASN
1	C	150	ASN
1	C	173	ASN
1	C	202	HIS
2	D	92	ASN
2	D	114	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	SCR	B	1	-	56,56,56	2.26	19 (33%)	79,92,92	2.03	21 (26%)
3	SCR	D	1	-	56,56,56	2.21	21 (37%)	79,92,92	2.19	23 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SCR	B	1	-	-	0/48/88/88	0/2/2/2
3	SCR	D	1	-	-	0/48/88/88	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	SCR	O5-C5	-3.12	1.36	1.44
3	D	1	SCR	O44-S4	-2.51	1.37	1.50
3	B	1	SCR	O3-C3	-2.49	1.41	1.46
3	D	1	SCR	O43-S4	2.02	1.52	1.45
3	D	1	SCR	O73-S13	2.02	1.52	1.45
3	B	1	SCR	O10-C12	2.04	1.47	1.42
3	B	1	SCR	O82-S11	2.05	1.52	1.45
3	B	1	SCR	O4-S4	2.08	1.63	1.57
3	D	1	SCR	O93-S12	2.08	1.52	1.45
3	D	1	SCR	O53-S14	2.09	1.52	1.45
3	B	1	SCR	O73-S13	2.11	1.52	1.45
3	D	1	SCR	O83-S11	2.14	1.53	1.45
3	B	1	SCR	O72-S13	2.21	1.53	1.45
3	D	1	SCR	O33-S3	2.31	1.53	1.45
3	B	1	SCR	O93-S12	2.34	1.53	1.45
3	B	1	SCR	O92-S12	2.34	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	SCR	O3-S3	2.44	1.64	1.57
3	B	1	SCR	O33-S3	2.44	1.54	1.45
3	B	1	SCR	C3-C2	2.55	1.57	1.52
3	D	1	SCR	O92-S12	2.55	1.54	1.45
3	B	1	SCR	C12-C13	2.58	1.58	1.54
3	B	1	SCR	O91-C13	2.81	1.54	1.47
3	D	1	SCR	O52-S14	2.89	1.55	1.45
3	D	1	SCR	O4-S4	3.18	1.67	1.57
3	D	1	SCR	O91-S12	3.33	1.67	1.57
3	B	1	SCR	O2-S2	3.39	1.68	1.57
3	D	1	SCR	O2-C2	3.48	1.53	1.46
3	D	1	SCR	O32-S3	3.51	1.58	1.45
3	D	1	SCR	C3-C2	3.75	1.60	1.52
3	D	1	SCR	O71-S13	3.88	1.69	1.57
3	D	1	SCR	O81-S11	3.89	1.69	1.57
3	D	1	SCR	O51-S14	4.49	1.71	1.57
3	D	1	SCR	C11-C12	4.73	1.57	1.52
3	D	1	SCR	O3-S3	4.93	1.72	1.57
3	B	1	SCR	O71-S13	5.02	1.73	1.57
3	B	1	SCR	O81-S11	5.14	1.73	1.57
3	B	1	SCR	O51-S14	5.15	1.73	1.57
3	D	1	SCR	O2-S2	5.46	1.74	1.57
3	B	1	SCR	O91-S12	6.10	1.76	1.57
3	B	1	SCR	C11-C12	6.24	1.59	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	SCR	O5-C5-C6	-4.33	97.75	106.61
3	D	1	SCR	O3-C3-C4	-4.03	99.58	108.48
3	D	1	SCR	O5-C1-C2	-3.33	102.77	109.47
3	D	1	SCR	C11-C12-C13	-3.30	107.85	115.31
3	D	1	SCR	O6-S6-O63	-2.99	97.50	106.77
3	B	1	SCR	C1-C2-C3	-2.80	104.86	110.75
3	B	1	SCR	C1-O5-C5	-2.31	109.25	113.75
3	D	1	SCR	C1-O5-C5	-2.18	109.51	113.75
3	D	1	SCR	O6-C6-C5	-2.12	103.83	107.90
3	B	1	SCR	O71-S13-O72	2.03	113.46	106.86
3	B	1	SCR	O91-S12-O93	2.08	113.63	106.86
3	B	1	SCR	O5-C5-C4	2.10	114.19	109.75
3	B	1	SCR	O51-S14-O53	2.11	113.33	106.77
3	B	1	SCR	O81-S11-O83	2.13	113.39	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	SCR	O10-C12-C11	2.26	112.81	107.59
3	D	1	SCR	O10-C12-C11	2.31	112.91	107.59
3	D	1	SCR	C3-C4-C5	2.32	115.59	110.55
3	D	1	SCR	O3-S3-O33	2.38	114.58	106.86
3	B	1	SCR	O6-S6-O62	2.53	114.63	106.77
3	B	1	SCR	O10-C15-C14	2.64	107.98	103.52
3	B	1	SCR	O4-S4-O43	2.64	115.44	106.86
3	B	1	SCR	O44-S4-O43	2.65	118.54	108.56
3	D	1	SCR	O71-S13-O73	2.69	115.59	106.86
3	D	1	SCR	O3-C3-C2	2.71	114.48	108.48
3	B	1	SCR	O91-C13-C14	2.78	117.76	108.80
3	D	1	SCR	O71-C14-C13	2.90	116.70	109.09
3	B	1	SCR	O10-C15-C16	2.95	116.21	109.49
3	D	1	SCR	O4-S4-O43	3.00	116.58	106.86
3	B	1	SCR	O2-C2-C3	3.08	115.29	108.48
3	D	1	SCR	O6-S6-O62	3.23	116.81	106.77
3	B	1	SCR	O71-C14-C13	3.45	118.14	109.09
3	D	1	SCR	C3-O3-S3	3.54	125.51	118.77
3	B	1	SCR	C3-O3-S3	3.65	125.72	118.77
3	B	1	SCR	C2-O2-S2	3.71	125.83	118.77
3	D	1	SCR	O91-C13-C14	3.86	121.25	108.80
3	B	1	SCR	O2-C2-C1	4.14	113.28	107.65
3	D	1	SCR	C4-O4-S4	4.15	126.67	118.77
3	D	1	SCR	O1-C1-C2	4.16	115.31	107.57
3	D	1	SCR	C2-O2-S2	4.99	128.27	118.77
3	D	1	SCR	C13-O91-S12	5.73	128.26	118.36
3	D	1	SCR	C14-O71-S13	5.88	129.96	118.77
3	B	1	SCR	C14-O71-S13	6.00	130.19	118.77
3	D	1	SCR	O2-C2-C3	6.53	122.93	108.48
3	B	1	SCR	C13-O91-S12	8.48	133.00	118.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	SCR	6	0
3	D	1	SCR	18	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	100/100 (100%)	-0.06	2 (2%) 68 63	4, 9, 15, 29	0
1	C	100/100 (100%)	0.03	2 (2%) 68 63	4, 9, 15, 23	0
2	B	128/131 (97%)	0.35	9 (7%) 19 13	2, 10, 17, 21	1 (0%)
2	D	131/131 (100%)	0.30	8 (6%) 25 18	5, 11, 17, 22	1 (0%)
All	All	459/462 (99%)	0.18	21 (4%) 36 29	2, 10, 17, 29	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	4.1
2	B	125	TYR	3.8
2	D	51	VAL	3.8
2	D	7	ASN	3.8
2	B	52	GLY	3.4
2	B	49	GLU	3.3
2	D	9	LYS	3.2
2	D	91	GLU	3.0
2	D	125	TYR	3.0
2	B	91	GLU	2.8
2	B	27	PRO	2.7
1	A	212[A]	GLN	2.6
2	B	101	LYS	2.5
2	D	8	TYR	2.4
2	B	50	SER	2.3
2	D	104	GLU	2.3
1	C	245[A]	HIS	2.3
2	B	88	ARG	2.2
2	D	90	GLU	2.2
1	C	197	GLU	2.1
1	A	245[A]	HIS	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SCR	B	1	55/55	0.82	0.24	0.63	73,94,114,115	0
3	SCR	D	1	55/55	0.83	0.21	0.01	71,92,114,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.